Lectures on Quantum Algorithms
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Basic facts about quantum mechanics. States of spin 1/2 particles

Vladimir S. Gerdjikov

Institute of Mathematics and Informatics
Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

Institute for Advanced Physical Studies, 111 Tsarigradsko chaussee, Sofia 1784, Bulgaria

`https://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation \\`
`https://physics.stackexchange.com/questions/477375/product-of-n-pauli-matrices`
`https://en.wikipedia.org/wiki/Ising_model`

Wolfgang Scherer. Mathematics of Quantum Computing.

Chapters 2& 3

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Notations:

Symbol	In my Lectures	In Scherer's book
w^*	complex conjugate of w	hermitian conjugate of w
$w^\dagger$	hermitian conjugate of w	not used
$\overline{w}$	not used	complex conjugate of w

The birth of quantum mechanics

Michelson experiment (1887) – the speed of light is independent on the direction it moves on.

The photo-effect Heinrich Hertz (1887) – emission of electrons when a metal is under electromagnetic radiation.

$$K_{\max} = \hbar(\nu - \nu_0).$$

where $K_{\max}$ is the maximum kinetic energy of the electrons, ν_0 is the minimum frequency at which the effect starts.

Explained by Einstein in 1905. In 1916 Millikan made an experiment which allowed him to measure the Plank constant:

$$\hbar = 6.5510^{-27} \quad \text{erg} \quad \text{sec}.$$

Light or electromagnetic radiations were thought and described as waves.

Einstein explained the photo-effect assuming that **the photons may behave as particles!**.

New ideas explaining the micro-world:

- **The energy of the waves and particles comes in quanta – Plank (1900):** $E = \hbar\nu$**;**
- **Waves may behave as particles and particles may behave like waves depending on the conditions or particle–wave dualism Louis de Brogle - (1924)**
- **Heisenberg uncertainty principle (1927):**

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2},$$

- **Description of the atomic and sub-atomic particles is based on Schrödinger equation. For a single particle with mass** m **in one dimension it is:**

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t).$$

where V is the potential of the media. The wave function $\Psi(t,x)$ determines the probability $|\Psi(x,t)|^2$ that the particle is at position x.

These ideas formed the basis of quantum mechanics.

Generic Schrödinger equation

Below we will assume that $\hbar = 1$ and $m = 1$.

$$i\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi(x,t)\rangle,$$

where $\hat{H}$ is an operator in the Hilbert space $\mathbb{H}$. $\hat{H}$ is known as the Hamiltonian of the system. Typically:

$$\hat{H} = -\Delta + V(x,y,x,t), \qquad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2},$$

where $V(x,y,z,t)$ is the potential of the media.

Static Schrödinger equation: if $\psi(x,t)\rangle = e^{-iEt}\psi(x)\rangle$ then:

$$\hat{H}|\psi(x)\rangle = E|\psi(x)\rangle,$$

where E is an eigenvalue of the Hamiltonian $\hat{H}$, or the energy of system.

Let A is an observable (some physical quantity of the particle). Then it is described by a hermitian (self-adjoint) operator in the Hilbert space $\mathbb{H}$ which in this case may be an infinite-dimensional one. The **mean value of the observable** A for the state $|\psi\rangle$ is provided by:

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle.$$

Using the fact that $A = \sum_j \lambda_j |e_j\rangle\langle e_j|$ we obtain:

$$\langle\psi|A|\psi\rangle = \langle\psi|\sum_j \lambda_j |e_j\rangle\langle e_j|\psi\rangle = \sum_j \lambda_j |\langle\psi|e_j\rangle|^2.$$

The possible values of the observable A are given by the eigenvalues λ_j of A (the spectrum of A).

For every normed $|\psi\rangle$ with $||\psi|| = 1$ the set

$$S_\psi \equiv \{e^{i\alpha}|\psi\rangle, \qquad \alpha \in \mathbb{R}\},$$

is called a ray in the Hilbert space $\mathbb{H}$ with $|\psi\rangle$ as a representative.

The uncertainty $\Delta_\psi(A)$ of measuring the observable A is defined by:

$$\Delta_\psi(A) = \sqrt{\langle\psi(A - \langle A\rangle_\psi)^2\psi\rangle} = \sqrt{\langle(A - \langle A\rangle_\psi)^2\rangle_\psi}.$$

If $\Delta_\psi(A) = 0$ then the value of the observable A in the state $|\psi\rangle$ is called **sharp**.

Two observables A and B are called compatible if $[A, B] = 0$. If $[A, B] \neq 0$ they are called incompatible.

If A and B are self-adjoint and if $[A, B] = 0$ then there exist an orthonormal basis $|e_j\rangle$ such that

$$A = \sum_j a_j|e_j\rangle\langle e_j|, \qquad B = \sum_j b_j|e_j\rangle\langle e_j|.$$

In particular this means that such A and B can be simultaneously taken to be diagonal.

It is possible to prove, that for any observables A and B and state $|\psi\rangle$ the following uncertainty condition holds:

$$\Delta_\psi(A)\Delta_\psi(B) \geq \left| \left\langle \frac{1}{2i}[A, B] \right\rangle_\psi \right|$$

Therefore, if $[A, B] = 0$ then $\Delta_\psi(A)\Delta_\psi(B) = 0$ and therefore a_j and b_j can be measured exactly.

The Heisenberg uncertainty relation:
Let the position operator Q_j and the momentum operator P_j be given by

$$|Q_j|\psi\rangle(\vec{x}) = |x_j\psi\rangle(\vec{x}), \qquad |P_j|\psi\rangle(\vec{x}) = \left|-i\frac{\partial}{\partial x_j}\psi\right\rangle(\vec{x}),$$

Check, that

$$[Q_j, P_k] = i\delta_{jk}\mathbb{1}$$

and therefore

$$\Delta_\psi(Q_j)\Delta_\psi(P_k) \geq \frac{1}{2}\delta_{jk}.$$

If a measurement of the observable A on the quantum mechanical system in the pure state $|\psi\rangle$ yields the eigenvalue λ then the measurement has effected the following state transition:

$$|\psi\rangle \qquad \Rightarrow \qquad \frac{P_\lambda|\psi\rangle}{||P_\lambda|\psi\rangle||},$$

where P_λ is the projector onto the eigensubspace of λ.

The measurement changes the wave-function of the state!

The quantum mechanics describes adequately numerous phenomena in the micro-world such as interatomic interactions, in solid state physics, statistical physics etc.

Spin models – the Ising model

The Ising model describes spin-spin interactions on a lattice. In general this could be lattice $\Lambda \in \mathbb{E}_d$ in d-dimensional space. We assume that the particles located at the each of the lattice sites k have spin $1/2$. We assume also that only the nearest neighbors interact, so that the Hamiltonian is given by:

$$H(S) = -\sum_{(i,j)} J_{ij} S_i S_j - \mu \sum_i h_j S_J, \qquad S_j \in \{1, -1\};$$

where (i, j) runs only on the nearest neighbors, J_{ij} is the strength of the interaction, μ is the magnetic moment=

The problem is to find the probability configuration:

$$P_\beta(S) = \frac{e^{-\beta H(S)}}{\mathbb{Z}_\beta}, \qquad \mathbb{Z}_\beta = \sum_S e^{-\beta H(S)},$$

where $\beta = (k_B T)^{-1}$ and k_B is the Boltzman constant.

Simplified Ising model:

$$H(S) = -J \sum_{(i,j)} S_i S_j.$$

If $J > 0$ these models describe ferromagnets; if $J < 0$ – antiferromagnets.

Pauli matrices and their tensor products

Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}_2.$$

Properties:

$$\sigma_k^2 = \sigma_0 = \mathbb{1}_2, \quad \sigma_k \sigma_j = i\epsilon_{kjm}\sigma_m, \qquad \{k, j, m\} = \{1, 2, 3\}$$

where ϵ_{jkm} is totally antisymmetric tensor, i.e.

$$\epsilon_{123} = 1, \qquad \epsilon_{kjm} = -\epsilon_{jkm} = \epsilon_{mkj}.$$

$$\sigma_1\sigma_2 = i\sigma_3, \quad \sigma_2\sigma_3 = i\sigma_1, \quad \sigma_2\sigma_1 = -i\sigma_3, \quad \sigma_3\sigma_2 = -i\sigma_1.$$

They appear when we need to describe the so-called spinor particles in quantum mechanics. An example of such particle is the electron which has spin 1/2. Pauli discovered that such particles may have only two states: the first one with spin up $|0\rangle$ and the second one with spin down $|1\rangle$. This nicely corresponds to the fact that in computers we use bites which also take two values.

Thus acting on bits we will have operators in $\mathbb{C}^2$ which are expressed in terms of Pauli matrices.

When we have two or more bites we will need tensor products of Pauli matrices:

$$\sigma_k \otimes \sigma_m, \qquad k, m = 0, 1, 2, 3;$$

These are 4×4 matrices of the form:

$$\sigma_0 \otimes \sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \qquad \sigma_1 \otimes \sigma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

$$\sigma_2 \otimes \sigma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}, \qquad \sigma_3 \otimes \sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix},$$

Examples and other possibilities for $\sigma_0 \otimes \sigma_1$:

$$\sigma_0 \otimes \sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \sigma_1 \otimes \sigma_0 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

Properties:

$$(cA) \otimes B = A \otimes (cB) = c(A \otimes B); \qquad (A \otimes B)(C \otimes D) = (AC) \otimes (BD).$$

We can construct also **triple tensor products** of Pauli matrices

$$\sigma_k \otimes \sigma_m \otimes \sigma_j, \qquad k, m, j = 0, 1, 2, 3;$$

They have dimension 8.

Properties:

$$(cA) \otimes B \otimes C = A \otimes (cB) \otimes C = A \otimes B \otimes (cC) = c(A \otimes B \otimes C);$$

$$(A \otimes B \otimes C)(F \otimes G \otimes H) = (AF) \otimes (BG) \otimes (CH)$$

Studying Ising models requires higher tensor products.

Thus analyzing the action of the processors on the bites we will need operators whose matrix dimensions will be powers of 2.